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# ME469: Advection Operators: Monotonicity Through “Unwinding” and “Limiters”

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## Dissipation and Dispersion Error: Review

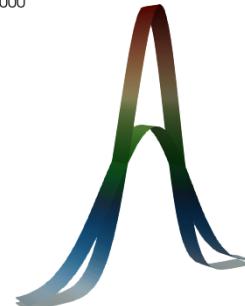
Recall, in our modified one-dimensional advection of a passive scalar, we had two types of errors that manifested depending on the underlying numerical approach:

- Dissipative-like error:

$$\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} - \alpha \frac{\partial^2 \phi}{\partial x^2} = 0$$

$$\phi(x, t) = e^{(-ivk - \alpha k^2)t} e^{ikx} = e^{ik(x-vt)} e^{-\alpha k^2 t}$$

Time: 2.000000

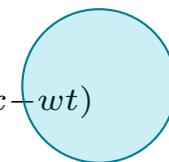


- Dispersion-like error:

$$\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} + \beta \frac{\partial^3 \phi}{\partial x^3} = 0$$

$$\phi(x, t) = e^{(-ivk + \beta ik^3)t} e^{ikx} = e^{ik[x-(v-\beta k^2)t]} = e^{ik(x-wt)}$$

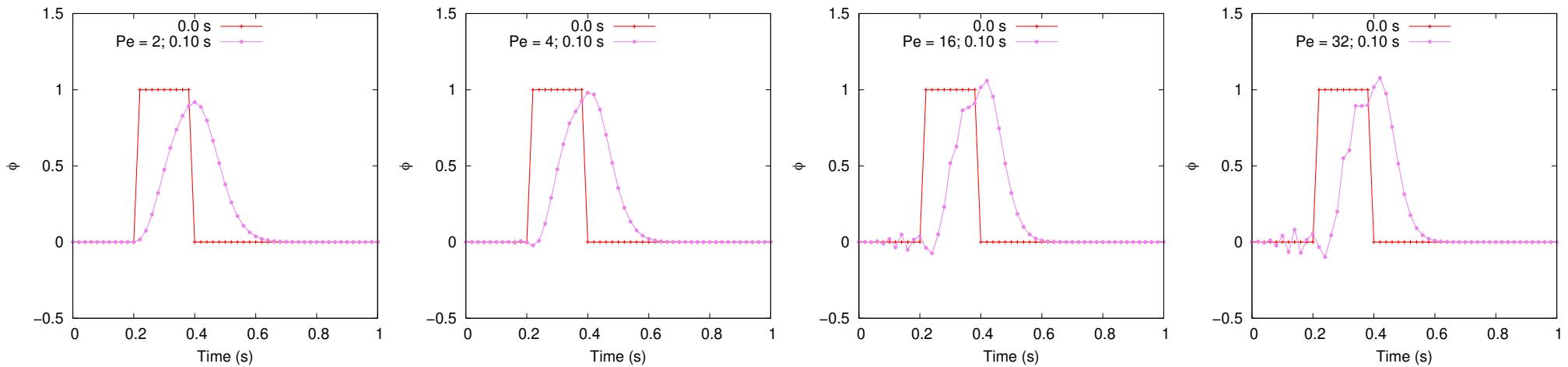
Time: 8.000000



## Transient Advection/Diffusion: Step Function as Initial Condition Central, AKA Galerkin

Goal: Run our model equation with a variety of Peclet numbers using a step function as the initial condition

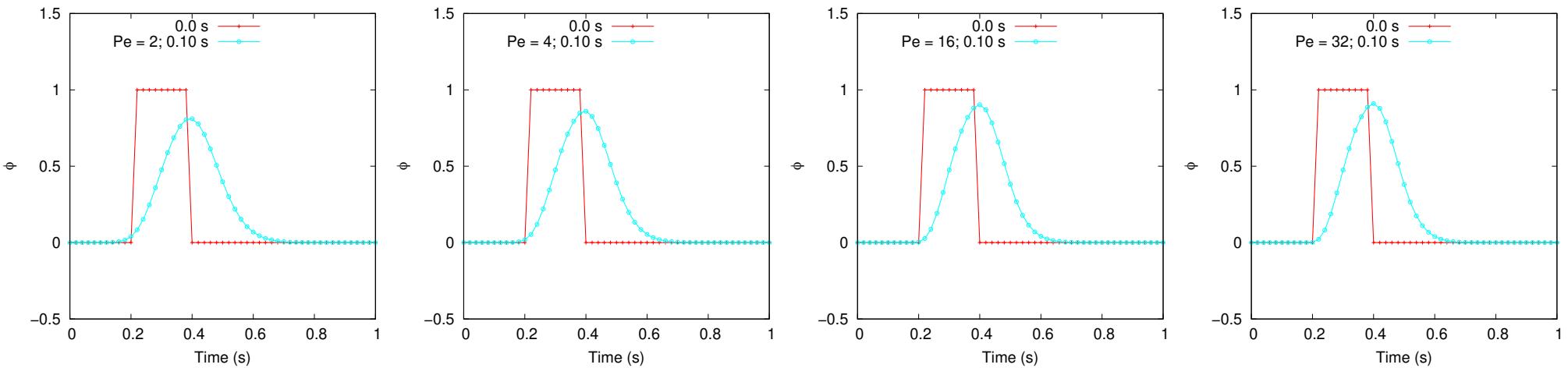
$$\int w \frac{\partial \rho u_j \phi}{\partial x_j} dV \approx \sum_{ip} (\rho u_j)_{ip} \phi_{ip} n_j dS \approx \sum_{ip} \dot{m}_{ip} \phi_{ip} \quad \phi_{ip}^{CDS} = \sum_n N_n^{ip} \phi_n$$



## Transient Advection/Diffusion: Step Function as Initial Condition First-order Upwind

Goal: Run our model equation with a variety of Peclet numbers using a step function as the initial condition

$$\dot{m}_{ip}\phi_{ip}^{UPW} = \frac{\dot{m} + |\dot{m}|}{2}\phi_L + \frac{\dot{m} - |\dot{m}|}{2}\phi_R$$





## Hybrid-Based Blending

For our general temporal advection/diffusion/source equation, can we define an improved, automatic blended approach between central and upwind?

$$\frac{\partial \rho\phi}{\partial t} + \frac{\partial \rho u_j \phi}{\partial x_j} - \frac{\partial}{\partial x_j} \left( \frac{\mu}{Sc} \frac{\partial \phi}{\partial x_j} \right) = S^\phi$$

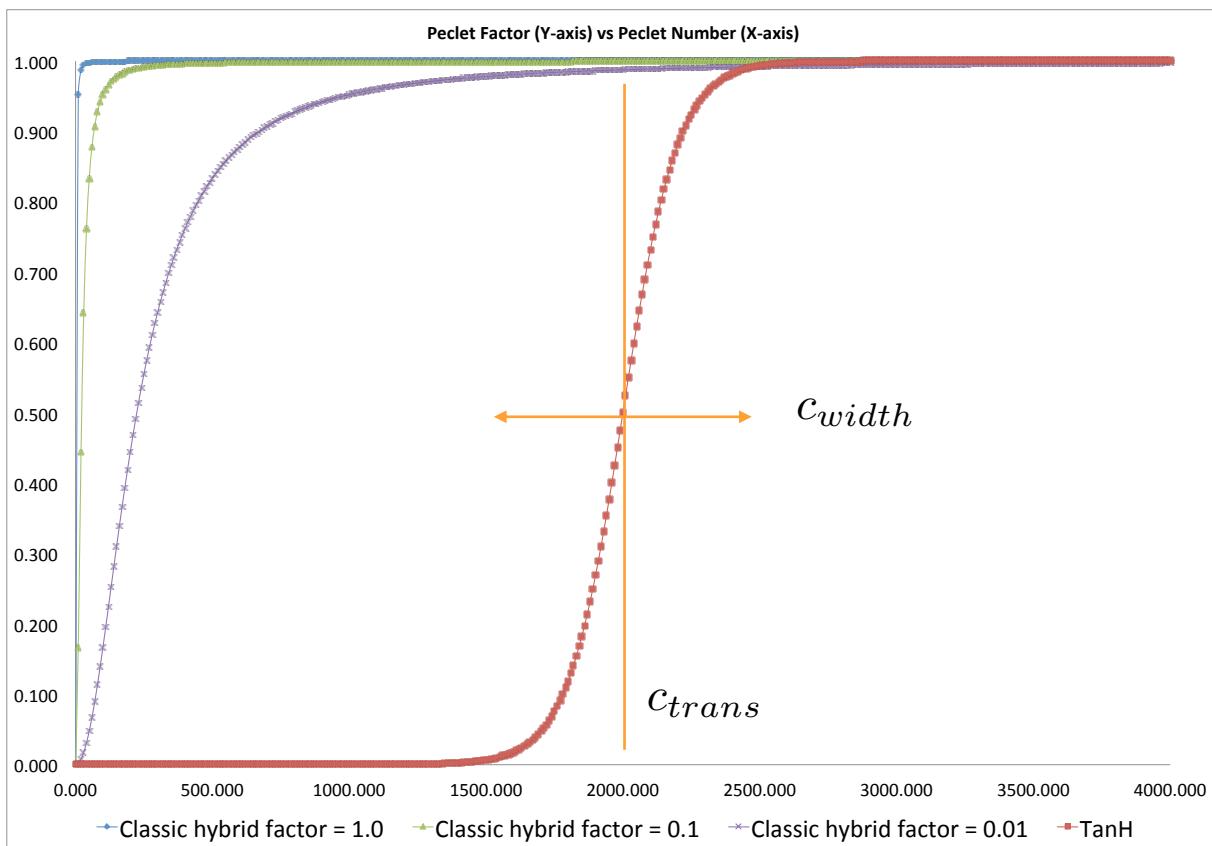
Recall, the advection operator was:  $\int w \frac{\partial \rho u_j \phi}{\partial x_j} dV \approx \sum_{ip} (\rho u_j)_{ip} \phi_{ip} n_j dS \approx \sum_{ip} \dot{m}_{ip} \phi_{ip}$

With (for central, or Galerkin):  $\phi_{ip}^{CDS} = \sum_n N_n^{ip} \phi_n$

And (for first-order upwind):  $\phi_{ip}^{FOU} = \frac{\dot{m} + |\dot{m}|}{2} \phi_L + \left| \frac{\dot{m} - |\dot{m}|}{2} \right| \phi_R$

We can define a blended operator as well:  $\phi_{ip} = \eta \phi^{FOU} + (1 - \eta) \phi^{CDS}$

## Functional form for $\eta$ – Linked to Peclet number, Pe Many ad-hoc choices, however, a common physical approach is tanh



$$Pe = \frac{\rho U L}{\mu}$$

$$\eta = \frac{1}{2} \left[ 1 + \tanh \left( \frac{Pe - c_{trans}}{c_{width}} \right) \right]$$

- peclet\_function\_form:
  - velocity: tanh
  - mixture\_fraction: tanh

- peclet\_function\_tanh\_transition:
  - velocity: 5000.0
  - mixture\_fraction: 2.0

- peclet\_function\_tanh\_width:
  - velocity: 200.0
  - mixture\_fraction: 4.0



## Hybrid-Blending Sanity Check

Consider a simple fluids case where we have air (298.15K) flowing 1 m/s in a 1 m<sup>3</sup> domain

- For  $\text{Pe} = 2$  at each element, we would require ~0.03 m resolution, or a mesh of size: ~35,000

Consider a simple fluids case where we have air (298.15K) flowing 10 m/s in a 1 m<sup>3</sup> domain

- For  $\text{Pe} = 2$  at each element, we would require ~0.003 m resolution, or a mesh of size: ~35,000,000
- In general, this constraint results in extremely high mesh counts for most all practical flow configurations; for turbulent regimes, we would quickly revert to  $\eta = \text{unity}$
- Moreover, as presented, we are blending with upwind – an operator that we have already shown to be overly diffuse and non-energy conserving



## Monotonic Issues at High Pe: Simple Matrix Analysis

Consider our passive scalar concentration whose natural range (as a mass fraction) is bounded between zero and unity, here, shown as a stationary transport equation:

$$\frac{\partial \rho u_j \phi}{\partial x_j} - \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial \phi}{\partial x_j} \right) = 0$$

Using our CDS and standard diffusion operator yields the following matrix system:

$$\left( \frac{\rho u}{2} [-1 \quad 0 \quad 1] + \frac{\rho D}{\Delta x} [-1 \quad 2 \quad -1] \right) \begin{bmatrix} \phi_{i-1} \\ \phi_i \\ \phi_{i+1} \end{bmatrix}. \quad a_{i,i-1} = \frac{\rho D}{\Delta x} \left( 1 + \frac{Pe}{2} \right)$$

With coefficients,  $a_{i,i}\phi_i = a_{i,i-1}\phi_{i-1} + a_{i,i+1}\phi_{i+1}$  and:  $a_{i,i} = (a_{i,i-1} + a_{i,i+1})$

Substituting:  $a_{i,i-1} = a_{i,i} - a_{i,i+1}$  and defining:  $\xi = \frac{a_{i,i+1}}{a_{i,i}}$   $a_{i,i+1} = \frac{\rho D}{\Delta x} \left( 1 - \frac{Pe}{2} \right)$

Yields:  $\phi_i = \xi\phi_{i+1} + (1 - \xi)\phi_{i-1}$  Positive for  $Pe < 2$

For  $Pe < 2$ , the value of the scalar at node  $i$  is a linear combination of the neighboring values

## Monotonic Issues Resolved When Using First-order Upwind

$$\frac{\partial \rho u_j \phi}{\partial x_j} - \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial \phi}{\partial x_j} \right) = 0$$



$$a_{i,i-1} = \frac{\rho D}{\Delta x} (1 + Pe)$$

Positive for all Pe

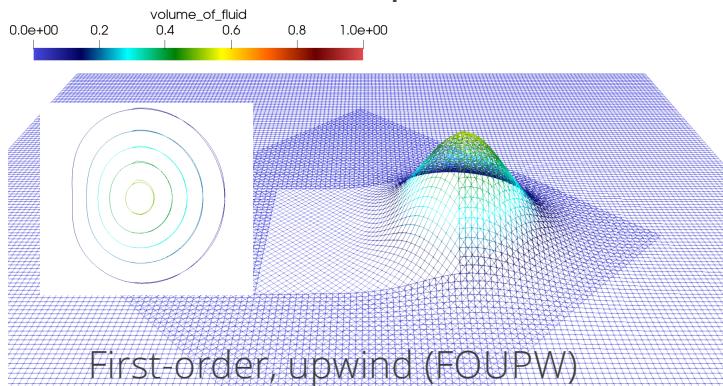
$$a_{i,i} = (a_{i,i-1} + a_{i,i+1})$$

$$a_{i,i+1} = \frac{\rho D}{\Delta x}$$

$$\left( \frac{\rho u}{2} [-1 \quad 1 \quad 0] + \frac{\rho D}{\Delta x} [-1 \quad 2 \quad -1] \right) \begin{bmatrix} \phi_{i-1} \\ \phi_i \\ \phi_{i+1} \end{bmatrix}$$

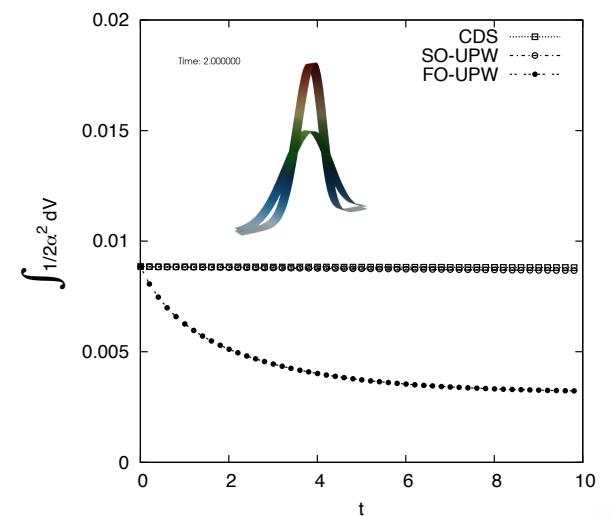
$$\phi_i = \xi \phi_{i+1} + (1 - \xi) \phi_{i-1} \quad \xi = \frac{a_{i,i+1}}{a_{i,i}}$$

However, at what price?

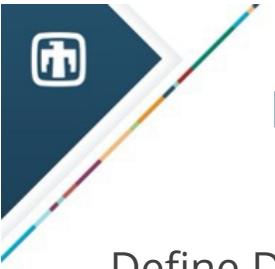


Fully bounded with diagonal dominance

$$\frac{\sum_{i \neq j} |a_{i,j}|}{|a_{i,i}|} \leq 1$$



Volume-of-fluid example (Domino and Horne, Renew. Ener. 2022)



## Monotonic Issues at high Pe: Alternative View (Diagonal Dominance)

Define Diagonal Dominance as:

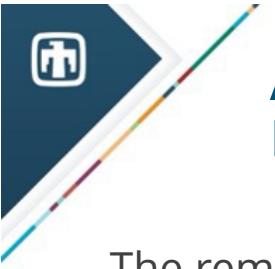
$$\frac{\sum_{i \neq j} |a_{i,j}|}{|a_{i,i}|} \leq 1$$

For a monotonic operator and ease of solving the linear system, diagonal dominance is desired

In our advection/diffusion case, this is expressed as:

$$\frac{|\frac{\rho D}{\Delta x} (1 - \frac{Pe}{2})| + |\frac{\rho D}{\Delta x} (1 + \frac{Pe}{2})|}{\frac{2\rho D}{\Delta x}} \leq 1$$

Which, again, is only ensured when the Peclet number is less than two



## Alternatives to First-order Upwind: Higher-order Upwind

The remaining set of slides are algebra-intensive!

- We do not intend for you to memorize these upcoming formulas, only the philosophy by which they are derived





## Alternatives to First-order Upwind: Higher-order Upwind

Recall, that in the finite difference context, we could increase the upwind stencil to increase accuracy, e.g.,

- For fluids: Varying reconstruction approaches:

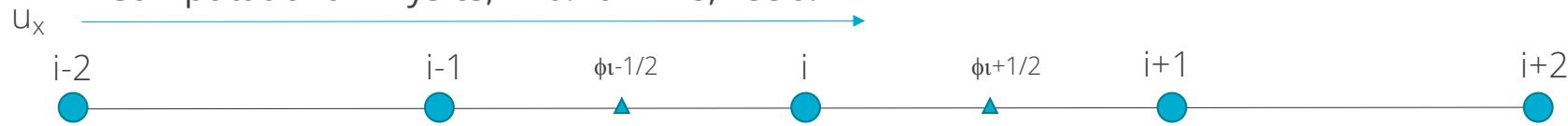
### *Essentially Non-oscillatory (ENO)*

- A. Harten, B. Engquist, S. Osher and S. Chakravarthy, Uniformly high order essentially non-oscillatory schemes, III, Journal of Computational Physics, 71:231-303, 1987.

### *Weighted-ENO (WENO)*

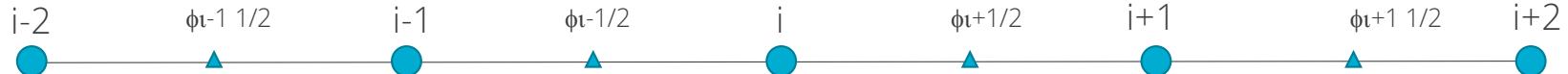
- 3<sup>rd</sup>-order, Liu, X., Osher, S. and Chan, T. (1994) Weighted Essentially Non-Oscillatory Schemes. Journal of Computational Physics, 115, 200-212.  
<https://doi.org/10.1006/jcph.1994.1187>
- Arbitrary-order, G. Jiang and C.-W. Shu, Efficient implementation of weighted ENO schemes, Journal of Computational Physics, 126:202-228, 1996.

Derivative	Accuracy	-8	-7	-6	-5	-4	-3	-2	-1	0
1	1								-1	1
	2							1/2	-2	3/2
	3						-1/3	3/2	-3	11/6





## ENO and WENO Concept



Define a suite of re-constructions that each provide 3<sup>rd</sup>-order accuracy:

$$\phi_{i+\frac{1}{2}}^{(1)} = \frac{1}{3}\phi_{i-2} - \frac{7}{6}\phi_{i-1} + \frac{11}{6}\phi_i \quad \phi_{i+\frac{1}{2}}^{(2)} = -\frac{1}{6}\phi_{i-1} + \frac{5}{6}\phi_i + \frac{1}{3}\phi_{i+1} \quad \phi_{i+\frac{1}{2}}^{(3)} = \frac{1}{3}\phi_i + \frac{5}{6}\phi_{i+1} - \frac{1}{6}\phi_{i+2}$$

- The above are simply defined by each of the three-point stencils, e.g.,
  - (i-2, i-1, i), (i-1, i, i+1) and (i, i+1, i+2)

We can also define a fifth-order scheme:

$$\phi_{i+\frac{1}{2}} = \frac{1}{30}\phi_{i-2} - \frac{13}{60}\phi_{i-1} + \frac{47}{60}\phi_i + \frac{9}{20}\phi_{i+1} - \frac{1}{20}\phi_{i+2}$$

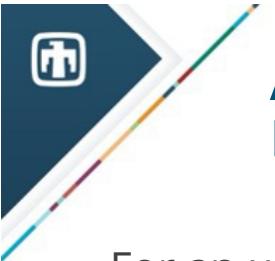
- This stencil can be reconstructed based on *linear weights*,  $\gamma$ :  $\gamma_1 = \frac{1}{10}, \gamma_2 = \frac{3}{5}, \gamma_3 = \frac{3}{10}$

$$\phi_{i+\frac{1}{2}} = \gamma_1 \phi_{i+\frac{1}{2}}^{(1)} + \gamma_2 \phi_{i+\frac{1}{2}}^{(2)} + \gamma_3 \phi_{i+\frac{1}{2}}^{(3)}$$

Or a convex-combination of weights: (sum to unity):

$$\phi_{i+\frac{1}{2}} = w_1 \phi_{i+\frac{1}{2}}^{(1)} + w_2 \phi_{i+\frac{1}{2}}^{(2)} + w_3 \phi_{i+\frac{1}{2}}^{(3)}$$

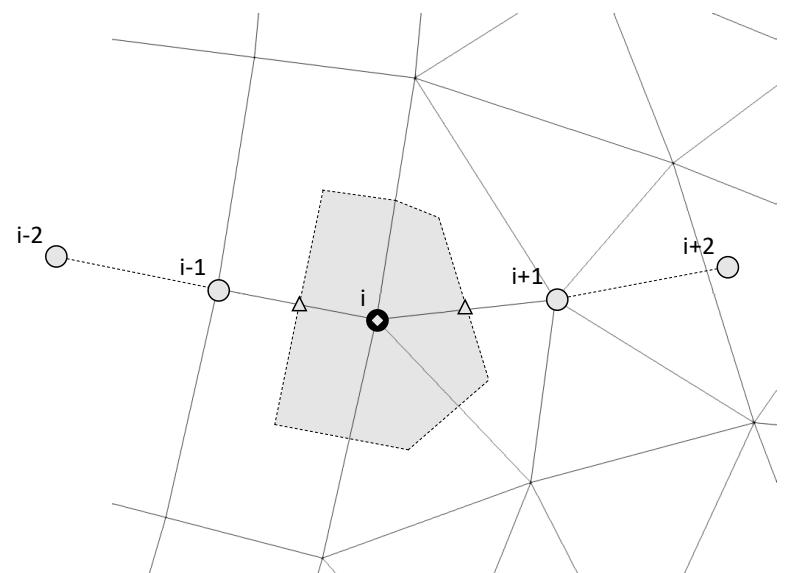
The weights,  $w_{1,2,3}$ , are a function of a “smoothness” factor ( $\beta_{1,2,3}$ ) that are dynamically selected

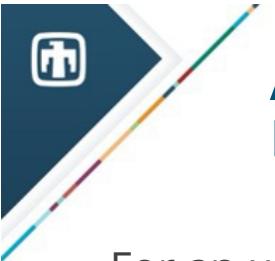


## Alternatives to First-order Upwind: Higher-order Upwind – But how on an unstructured mesh?

For an unstructured setting, the former approach is not easily achieved due to the reduced stencil connectivity

- Recall, we are looping edges (as shown), or elements
- How to proceed with reconstructing data that is outside the immediate connectivity?
- Ideas?

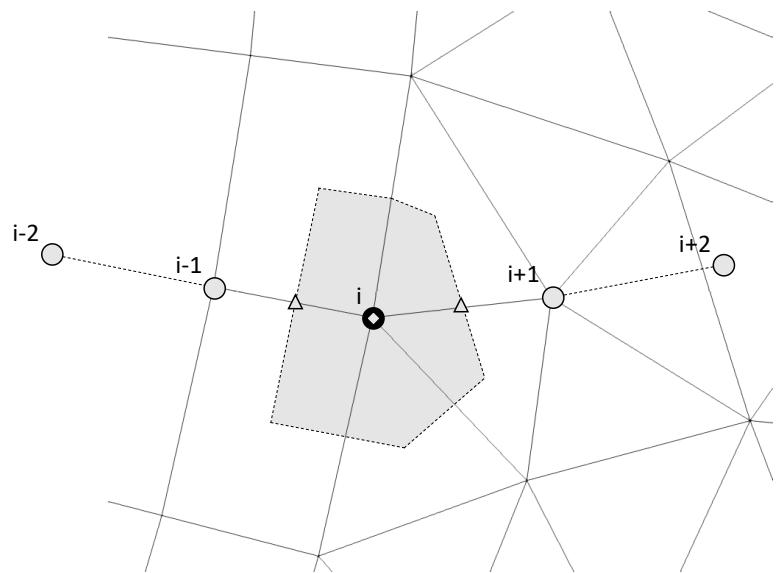




## Alternatives to First-order Upwind: Higher-order Upwind – But how on an unstructured mesh?

For an unstructured setting, the former approach is not easily achieved due to the reduced stencil connectivity

- Recall, we are looping edges (as shown), or elements
- How to proceed with reconstructing data that is outside the immediate connectivity?
- Ideas?
- Hint... Can we look towards the projected nodal gradient to effectively increase the stencil?





## General Kappa-Method of Hirsh

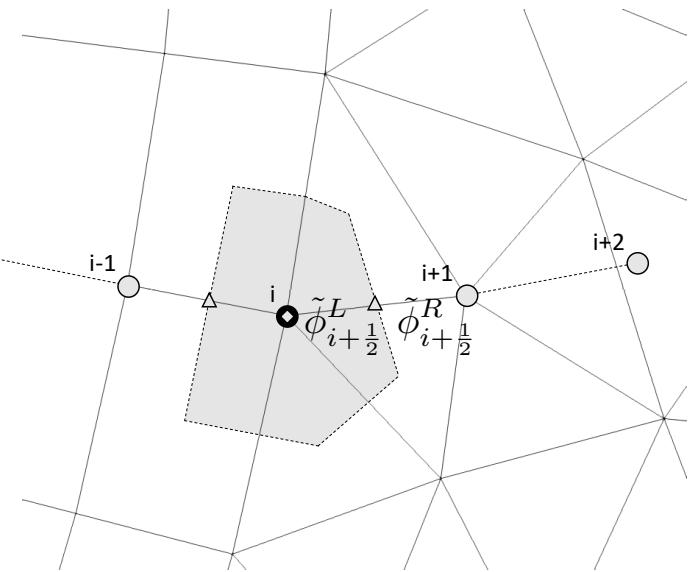
Numerical Computation of Internal and External Flows, vol. 2, John Wiley & Sons, 1990

For the edge defined by the  $i$  and  $i+1$  node, define a Left and Right state:

$$\tilde{\phi}_{i+\frac{1}{2}}^L = \phi_i + \frac{1}{4} [(1 - \kappa) (\phi_i - \phi_{i-1}) + (1 + \kappa) (\phi_{i+1} - \phi_i)],$$

$$\tilde{\phi}_{i+\frac{1}{2}}^R = \phi_{i+1} - \frac{1}{4} [(1 + \kappa) (\phi_{i+1} - \phi_i) + (1 - \kappa) (\phi_{i+2} - \phi_{i+1})].$$

- For  $\kappa = +1$ , we simply revert to CDS
- For  $\kappa = -1$ , Second-order upwind
- For  $\kappa = 2/3$ , QUICK (Leonard, "A stable and accurate convective modelling procedure based on quadratic upstream interpolation", Comput. Methods Appl. Mech. Eng. 19 (1979) 59–98.)



Assignment: Algebra!!!



## Kappa = 0 Method of Hirsh

Numerical Computation of Internal and External Flows, vol. 2, John Wiley & Sons, 1990.

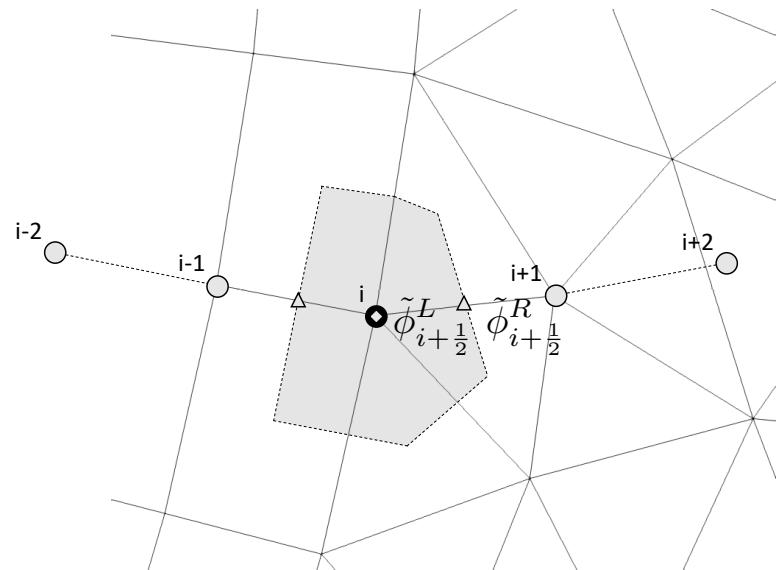
- For  $\kappa = 0$ , recast as: (Algebra....)

$$\tilde{\phi}_{i+\frac{1}{2}}^L = \phi_i + \Phi^L \Delta x_j^L G_j \phi_i,$$

$$\tilde{\phi}_{i+\frac{1}{2}}^R = \phi_{i+1} - \Phi^R \Delta x_j^R G_j \phi_{i+1}$$

Where,  $\Delta x_j^L = x_j^{ip} - x_j^L$ ,  
 $\Delta x_j^R = x_j^R - x_j^{ip}$

- Above, define a “limiter” function  $\Phi^L, \Phi^R$  that “senses” when the solution is smooth (tends towards unity) and when the solution is oscillatory (tends towards zero)
- $G_j$  is the projected nodal gradient at each node (or cell-center) that is treated in a *deferred-correction* context, i.e., this quantity is lagged from the previous iteration
- So-called “gradient reconstruction” schemes
  - Reconstruct a higher-order stencil through extrapolation



Derived by substituting  $\kappa = 0$ , and using the projected nodal gradient definition – or – just by noting an extrapolation using a gradient

Assignment: Algebra!!!



## Projected Nodal Gradient Refresher

- First, the gradient of a function (other than linear) is discontinuous, i.e., the value at a shared element face depends on which element is used to compute the gradient
- Therefore, we can view the nodal gradient as continuous at the nodes and discontinuous within the elements

Let's minimize this difference:

by solving:



## Projected Nodal Gradient: Refresher

- First, the gradient of a function (other than linear) is discontinuous, i.e., the value at a shared element face depends on which element is used to compute the gradient
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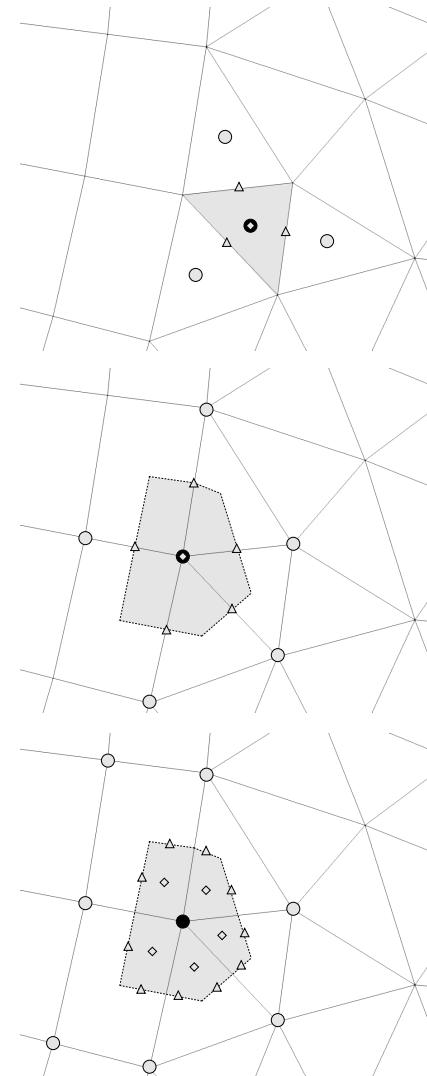
Let's minimize this difference:

$$\frac{1}{2} \left( \frac{\partial \phi}{\partial x_j} - G_j \phi \right)^2$$

by solving:

$$\int w G_j \phi dV = \int w \frac{\partial \phi}{\partial x_j} dV \rightarrow G_j \phi = \frac{\sum_{ip} \phi_{ip} n_j dS}{V}$$

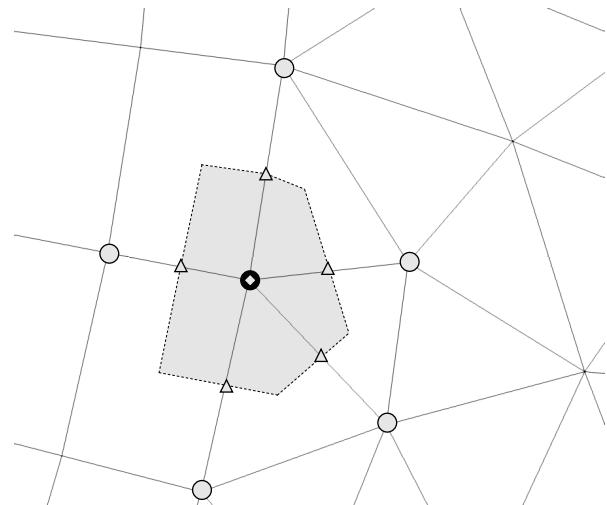
Lumped projected nodal gradient



## Projected Nodal Gradient: Psuedo Code (Edge-based)

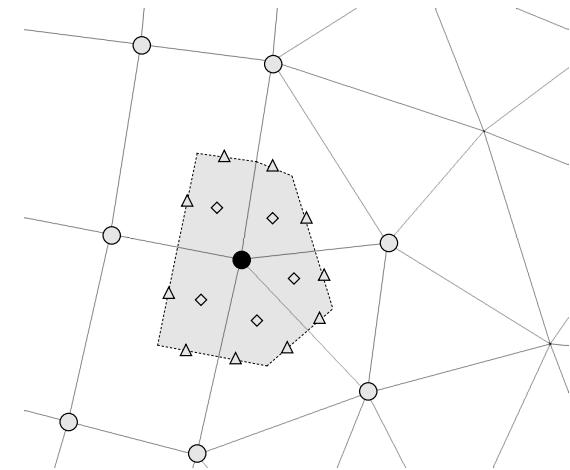
```
for ( stk::mesh::Bucket::size_type k = 0 ; k < length ; ++k ) {
    stk::mesh::Entity nodeL/nodeR = edge_node_rels[0]/edge_node_rels[1];
    const double qL = *stk::mesh::field_data( *scalarQ_, nodeL );
    const double qR = *stk::mesh::field_data( *scalarQ_, nodeR );
    const double qip = 0.5*(qL + qR);
    const double invVolL = 1.0/volL;
    const double invVolR = 1.0/volR;

    for ( int j = 0; j < nDim; ++j ) {
        const double aj = areaVector[k*nDim];
        gradQL[j] += aj*qip *invVolL;
        gradQR[j] -= aj*qip*invVolR;
    }
}
```



## Projected Nodal Gradient: Psuedo Code (CVFEM)

```
for ( int ip = 0; ip < numScsIp_ ; ++ip ) { // assemble to il/ir  
    // left and right nodes for this ip  
    const int il = lrscv[2*ip];  
    const int ir = lrscv[2*ip+1];  
  
    double qIp = 0.0;  
    const int offSet = ip*nodesPerElem_;  
    for (int ic=0; ic < nodesPerElem; ++ic ) {  
        qIp += N[offSet+ic]*p_scalarQ[ic];  
    }  
  
    for ( int j = 0; j < nDim_ ; ++j ) {  
        double fac = qIp*areaVec[ip*nDim_+j];  
        gradQL[j] += fac*inv_voll;  
        gradQR[j] -= fac*inv_volR;  
    }  
}
```





## Kappa = 0 Method of Hirsh: CVFEM

Numerical Computation of Internal and External Flows, vol. 2, John Wiley & Sons, 1990.

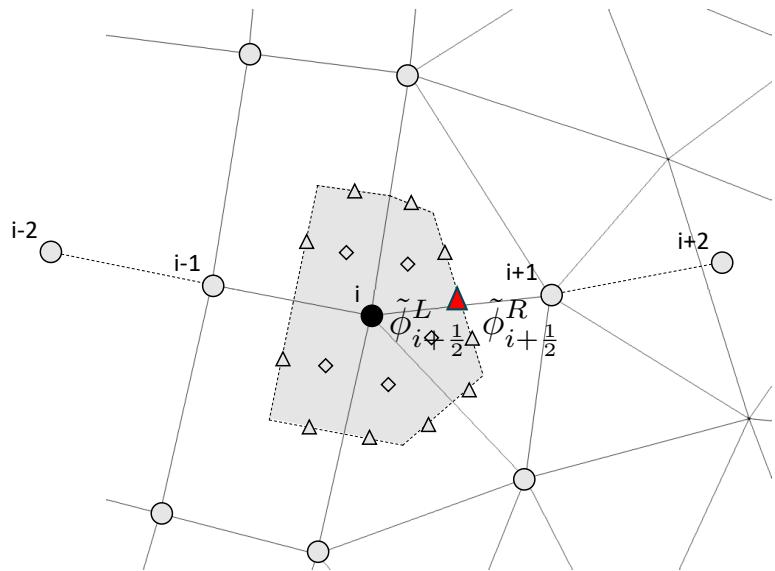
- For  $\kappa = 0$ , recast as: (Algebra.....)

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Where,  $\Delta x_j^L = x_j^{ip} - x_j^L$ ,  
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- So-called “gradient reconstruction” schemes
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CVFEM surface integration point can be along the edge, or at the standard SCS location with modified distance vector

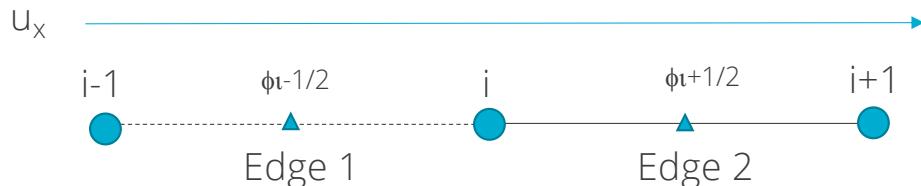
Assignment: Algebra!!!



## Classic Flux Limiters

Van Leer, B. (1974), "Towards the ultimate conservative difference scheme II. Monotonicity and conservation combined in a second order scheme", J. Comput. Phys., 14 (4): 361–370

- Consider our standard three-point stencil obtained by iterating edge 1 and 2



- In the above stencil, we are stressing that when iterating edge 2, we do not have information easily obtain for edge 1 (shown above as a dashed line); (speaking from an unstructured perspective)

$$\phi_{i+\frac{1}{2}} = \phi_{i+\frac{1}{2}}^{LOW} - \Phi(r_{i+\frac{1}{2}}) (\phi_{i+\frac{1}{2}}^{LOW} - \phi_{i+\frac{1}{2}}^{HIGH}) \quad \text{Monotonic upstream-centered scheme for conservation laws (MUSCL)}$$

- Above, the "LOW" and "HIGH" are any operators that you select, e.g.,

$$\phi_{i+\frac{1}{2}}^{LOW} = \phi_i \quad \phi_{i+\frac{1}{2}}^{HIGH} = \frac{\phi_i + \phi_{i+1}}{2} \rightarrow \phi_{i+\frac{1}{2}} = \phi_i + \frac{1}{2} \Phi(r_{i+\frac{1}{2}}) (\phi_{i+1} - \phi_i)$$

$$r_{i+\frac{1}{2}} = \frac{(\phi_i - \phi_{i-1})}{(\phi_{i+1} - \phi_i)} \quad (\phi_i - \phi_{i-1}) = 2G_x \phi_i \Delta x - (\phi_{i+1} - \phi_i) \quad G_x \phi_i = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}$$



## Flux Limiter Definition

Sweby (1984) defined set of permissible limiter regions for the desired second-order accurate methods: A sampling of the Sweby Diagram

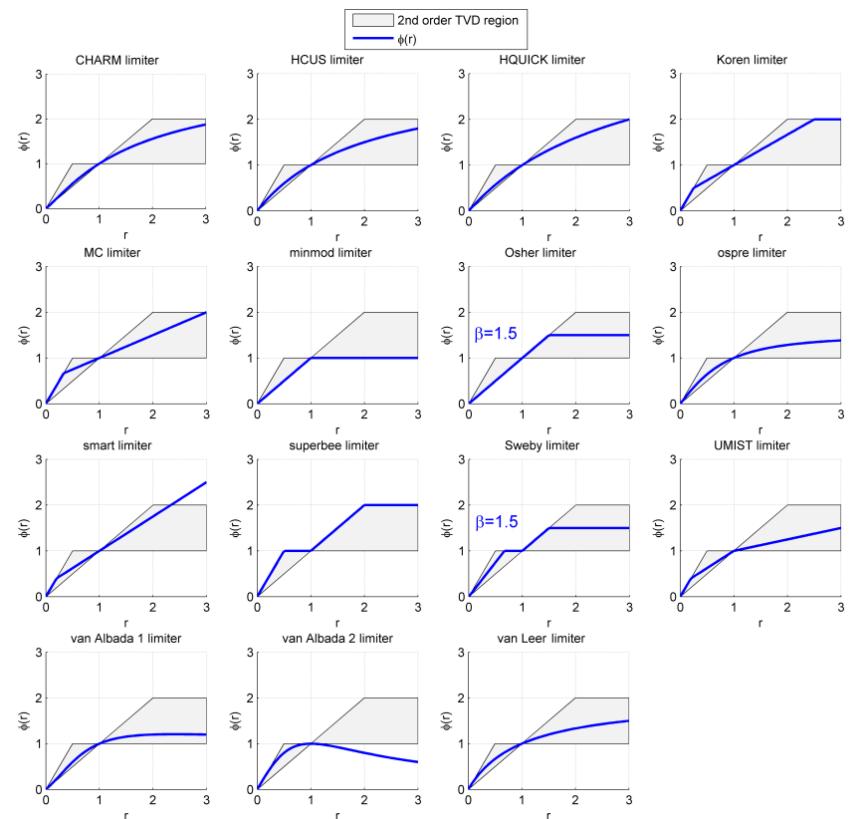
$$\text{Superbee: } \Phi(r) = \max[0, \min[2r, 1], \min[r/2]]$$

$$\text{Van Leer: } \Phi(r) = \frac{r + |r|}{1 + |r|}$$

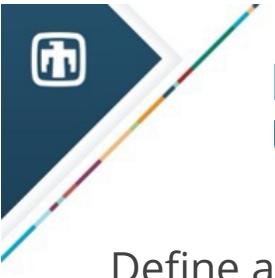
$$\text{Symmetry property: } \Phi(1/r) = \frac{\Phi(r)}{r}$$

$$\text{Total Variation: } TV(\phi) = \sum_{j=1}^N |\phi_j - \phi_{j-1}|$$

- For a monotonically increasing function,  $TV(\phi) = |\phi_1 - \phi_N|$ . Note that if  $\phi_1$  and  $\phi_N$  are taken constant, then, as long as the function remains monotonic the total variation is constant
- However, if  $TV(\phi)$  increases, then this suggest oscillations in the solution have occurred



Sweby's 2nd order TVD region. Created in Matlab. [Griffgruff](#) 18:37, 11 October 2006 (UTC)



## Blending Approaches to Arrive at Pseudo Higher-order Methods: Upwind and Central

Define an upwind operator now at an arbitrary integration point:

$$\begin{aligned}\phi_{ip}^{UPW} &= \alpha_{upw} \tilde{\phi}_{ip}^L + (1 - \alpha_{upw}) \phi_{ip}^{CDS}; \dot{m} > 0, \\ &\alpha_{upw} \tilde{\phi}_{ip}^R + (1 - \alpha_{upw}) \phi_{ip}^{CDS}; \dot{m} < 0.\end{aligned}$$

And for a generalized CDS scheme:

$$\begin{aligned}\phi_{ip}^{GCDS} &= \frac{1}{2} \left( \hat{\phi}_{ip}^L + \hat{\phi}_{ip}^R \right), & \hat{\phi}_{ip}^L &= \alpha \tilde{\phi}_{ip}^L + (1 - \alpha) \phi_{ip}^{CDS}, \\ && \hat{\phi}_{ip}^R &= \alpha \tilde{\phi}_{ip}^R + (1 - \alpha) \phi_{ip}^{CDS}\end{aligned}$$

- Two new blending parameters:  $\alpha_{upw}$  and  $\alpha$



## The Idealized Stencil Set

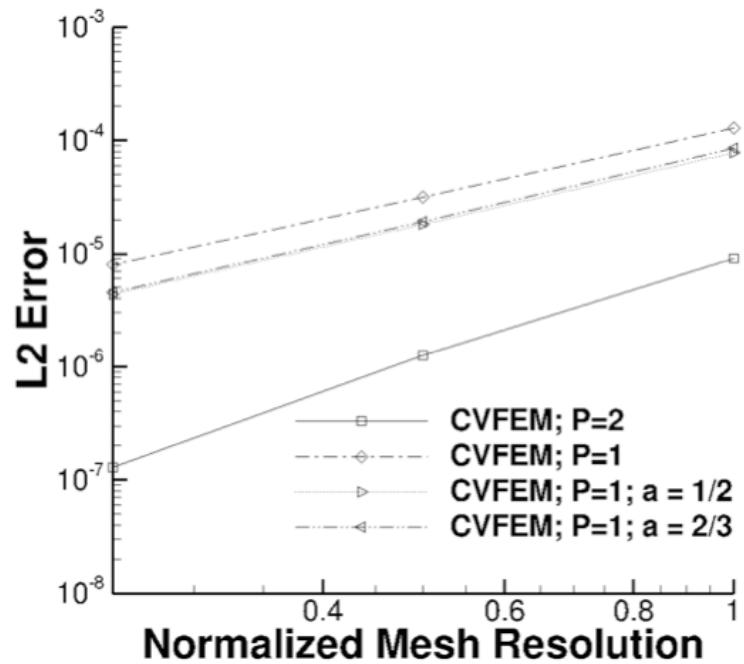
With Nalu input file specifications

$i - 2$	$i - 1$	$i$	$i + 1$	$i + 2$	$\alpha$	$\alpha_{upw}$
0	$-\frac{1}{2}$	0	$+\frac{1}{2}$	0	0	n/a
$+\frac{1}{8}$	$-\frac{6}{8}$	0	$+\frac{6}{8}$	$-\frac{1}{8}$	$\frac{1}{2}$	n/a
$+\frac{1}{12}$	$-\frac{8}{12}$	0	$+\frac{8}{12}$	$-\frac{1}{12}$	$\frac{2}{3}$	n/a
$+\frac{1}{4}$	$-\frac{5}{4}$	$+\frac{3}{4}$	$+\frac{1}{4}$	0	$\dot{m} > 0$	1
0	$-\frac{1}{4}$	$-\frac{3}{4}$	$+\frac{5}{4}$	$-\frac{1}{4}$	$\dot{m} < 0$	1
$+\frac{1}{6}$	$-\frac{6}{6}$	$+\frac{3}{6}$	$+\frac{2}{6}$	0	$\dot{m} > 0$	$\frac{1}{2}$
0	$-\frac{2}{6}$	$-\frac{3}{6}$	$+\frac{6}{6}$	$-\frac{1}{6}$	$\dot{m} < 0$	$\frac{1}{2}$

- alpha\_upw:  
velocity: 1.0
- alpha:  
velocity: 1.0
- upw\_factor: (zero reverts to first-order)  
velocity: 1.0
- limiter:  
velocity: [yes/no]

## Pseudo 4<sup>th</sup> order Verification Results

Verification using Central (linear and quadratic) compared to pseudo 4<sup>th</sup> order



Lower error, however, formally second-order accurate